

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) er022

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

## Datablock: er022

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Bond precision:	C-C = 0.0049 Å	Wavelength=0.71073
Cell:	a=9.9681(3)	b=15.9931(6)      c=16.2939(6)
	alpha=90	beta=92.160(3)      gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	2595.74(16)	2595.74(16)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	2(C16 H8 Li O8 Zn), 2(C0.75 H1.75 N0.25 O0.25), 2(C0.75 H1.75 N	?
Sum formula	C41 H42 Li2 N4 O17 Zn2	C41 H42 Li2 N4 O17 Zn2
Mr	1007.45	1007.40
Dx, g cm <sup>-3</sup>	1.289	1.289
Z	2	2
Mu (mm <sup>-1</sup> )	0.990	0.990
F000	1036.0	1036.0
F000'	1037.64	
h,k,lmax	13,21,22	12,20,20
Nref	6864	5802
Tmin,Tmax	0.779,0.837	0.898,1.000
Tmin'	0.750	

Correction method= # Reported T Limits: Tmin=0.898 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.845      Theta(max)= 28.926

R(reflections)= 0.0536( 4603)      wR2(reflections)= 0.1717( 5802)

S = 1.093      Npar= 406

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.



### Alert level C

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	012	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	032	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Zn1	Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N2N --H2NA .	Please	Check
PLAT420_ALERT_2_C	D-H Without Acceptor	N2N --H2NB .	Please	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....		3.244	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	27	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF ....		4	Note
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.81A From Old	0.43	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H2NB		-0.42	eA-3



### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		16	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		19	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3	Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....		4	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		5	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records		1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O1D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl1D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl2D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl3D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12E	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12F	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C23D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22D	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22E	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22F	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23C	Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2AA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2AB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2AC	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N1N	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl1N	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl2N	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1NA	Constrained at	0.5	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H1NB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2N	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21N	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22N	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2NA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2NB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22C	Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6 )		100%	Note
PLAT411_ALERT_2_G	Short Inter H...H Contact H37 ..H21D .		2.14	Ang.
	-1/2+x,1/2-y,-1/2+z =		4_565	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H21B ..H36 .		1.90	Ang.
	1/2+x,1/2-y,1/2+z =		4_666	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O12 ..C11N		2.90	Ang.
	3/2-x,-1/2+y,3/2-z =		2_646	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		7	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....		!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		220	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		885	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		15	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		2.2	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ		2	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ		2	Units
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities .....		Please	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		3	Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 79 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 6 ALERT type 3 Indicator that the structure quality may be low  
 63 ALERT type 4 Improvement, methodology, query or suggestion  
 5 ALERT type 5 Informative message, check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### **Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### **Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

